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NEUTRONIC AND THERMALHYDRAULIC ASPECTS - PWR APPLICATIONS

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1. NEUTRONIC AND THERMALHYDRAULIC ASPECTS FOR DESIGN AND OPERATION OF PWR

The main challenges emerging in the field of Reactor Physics in the past decade and requiring the continuous improvement of the nuclear data bases, the computer codes, and their extensive qualification, are connected to :

- the increase of the discharge burnup;
- the modifications in cycle length and the need for flexibility, leading to the introduction of advanced burnable poisons;
- the load following mode of operation and the associated patterns for control rod clusters;
- the recycling of MOX fuel;
- the criticality safety during outpile management of the fuel;
- the increased attention paid to the minor actinides, their production and their potential for transmutation in the reactors.

Among these problems, the MOX recycling includes the main difficulties concerning heterogeneities, self-shielding of the resonances, accuracy of the cross-sections, detailed isotopic composition. MOX recycling provided a very interesting benchmark for advanced models and codes.

2. INTRODUCTION

Precise computation of neutron flux in the core of a nuclear reactor represents one of the basic aspects of reactor design and operation. Neutron flux is computed by solving Boltzmann's linear equation. Anyway, the direct solution of the equation involves too great a number of operations for practical application, leading up to TeraFlops or even PetaFlops supercomputing capabilities.
Physical and mathematical models are then required to handle the extensive variety of configurations encountered. Numerical methods must be adapted to the rapid evolution of computer power, as also computer architecture : sequential, vector or parallel. Physical and mathematical models must allow for very fast estimation for on-line control and monitoring, adequate quantification for industrial studies and high-precision, best estimate computations.
Coupling of neutronics to mechanics and two-phase flow thermalhydraulics must be implemented in order to improve the accuracy in best-estimate computation schemes and to take into account the transient behaviour of the plant during normal operation or incidents.
In this field of continuous improvement, the new methods applied in Reactor Physics lead obviously to good results and provide the improvements required in the future for the needs of efficiency, safety and advanced fuel cycle.
This trend and the "evolutionary" implementation in large and modular software systems will be illustrated by the example of the SAPHYR system.

3 - THE SAPHYR SYSTEM

3.1 Purpose

The SAPHYR system was designed to provide an answer to neutronic computation needs in the electronuclear and naval propulsion fields, experimental or dedicated reactors of the CEA, etc. The system deals with several steps of the fuel cycle, including reactor core management and fuel cycle plants needs under normal and accidental operating conditions, including reactivity accidents. The system currently integrates in two steps assembly and core computation functions, including the neutronic-thermalhydraulic coupling

at the core level. The SAPHYR system is based on the modularity of the functions handled, a multi-level modelling strategy, extensive integration of new methods and solvers, in order to create a powerful, flexible and evolutive tool.

The nucleus of the SAPHYR system comprises the tightly coupled APOLLO2, CRONOS2, FLICA4 and PEPIN codes.

The APOLLO2 code computes the neutron flux in transport for extended configurations : cell, macrocell, assembly, lattices extending over several assemblies, interfaces and small isothermal cores. APOLLO2 combines collision probability (Pij) and discrete ordinates (Sn) methods. Equivalence procedures are used to switch from one method to the other, from transport to diffusion, and to homogenize the lattices.

Current development is concerned with processing PWR voided configurations, thus adapting APOLLO for rapid spectra. Other development work concerns kinetics and highly discretized energy computation (about 10000 groups as an order of magnitude).

The CRONOS2 kinetics code is designed for diffusion and transport core computation. This code includes a number of varied options, ranging from 3D "cell by cell" computation to computation using wide homogenized elements. CRONOS2 uses finite difference, finite elements and nodal solution methods. CRONOS2 can perform 3D transport core computation with discrete ordinates, for xyz or hexagonal geometries. This code is designed for management and operating studies, and can provide in this context best estimate or industrial computational schemes.

CRONOS2 incorporates its own simplified thermalhydraulic model, and is also coupled to FLICA4, or directly to FLICA S (see below).
CRONOS2 incorporates advanced core control methods, of potential interest for the PWR reactors of the future.

FLICA4 is a 3D core thermalhydraulic code designed for two-phase transient problems, and is an essential asset of the SAPHYR system for complex accident situations. FLICA4 incorporates FLICA S, which describes the behaviour of the primary coolant system.

The PEPIN code quantifies residual power, which is of fundamental importance in the safety context.

New lines of study appeared recently for integration in the objectives of the SAPHYR system, including for instance :

- degraded cores, corium, and low pressure criticality accidents,
- downstream end of the fuel cycle, and various methods of transmutation and incineration,
- extension to fusion-related studies.

3.2. Organization of the SAPHYR system

Each code incorporates a set of modules, each module providing a simple mathematical or physical function. The codes are interfaced by means of standard data structures, leaving each code to optimize its internal organization.

GIBIANE is the control language common to all SAPHYR system modules. The modularity of each code, code interconnection, and the GIBIANE module chaining language, provide an exceptional degree of functional flexibility, adapting to any type of studies, and also to industrial applications through a set of dedicated procedures.

3.3. Computation steps

The neutron flux in a reactor is determined by solving Boltzmann's linear equation.

The flux function involves 7 variables, namely 3 spatial variables, 2 angular variables, 1 energy variable and time. Two method categories are available for solving a problem of this type, namely determinist methods based on numerical discretization of the equation, and probabilist techniques involving the use of Monte Carlo methods.

At the present time, determinist computation methods are used predominantly for power reactors, this being principally due to the relatively periodic and repetitive nature of the core. This allows computation with different scales, using equivalence processes between the different levels.

The breakdown procedure currently used involves three levels. First the cross-section level, with extremely fine energy representation, then the assembly level, using about 100 energy groups for 2D transport modelling, and the final, core computation level, for which 3D diffusion approximation techniques are mainly used at the present time.

Estimation has demonstrated that we are still far from achieving complete, direct and detailed solution of Boltzmann's equation. Taking discretization of the core into 300 x 200 x 100 basic cells, with each cell represented by about 10 computation points, discretization into 100 angular directions, 10,000 energy groups and 100 time steps, and assuming finite difference approximation, requiring about 15 floating point operations per element, 5 internal iterations and 100 external iterations, we obtain a total of the order of 7.10^{18} floating point operations. This represents about 30 years of computation for a contemporary computer with a capacity of several Gigaflops. Furthermore, allowance must also be made for a detailed thermohydraulic configuration, and computation of cross-sections.

4. DEVELOPMENT CONTEXT

Insofar as PWR reactors are concerned, potential users for the SAPHYR system are CEA, EDF and FRAMATOME. FRAMATOME uses the APOLLO2 code as an essential link in its new SCIENCE computation system. EDF has been using APOLLO1 for several years, and has initiated a modernization programme for its core computation system, where APOLLO2 will play a primordial role.
At the core computation level, the tightly coupled CRONOS2 and FLICA4 are considered as reference codes, primarily oriented towards detailed transport and high-precision computation, and featuring new computation schemes which will be introduced in the industrial toolkits of the near future (whole core transport nodal and fine 3D computation, parallelism, etc.)
CRONOS represents a major link in the qualification of APOLLO and its nuclear data.

For the fuel cycle field, in connection with COGEMA, projects concerning extended development of the SAPHYR system in the area of criticality safety take shape through the CRISTAL toolkit, based on the SAPHYR and PROMETHEE (radiation transport, shielding) systems. SAPHYR and PROMETHEE provide also the basis for DARWIN, dedicated to fuel depletion, isotopic composition, source term and residual heat source. JEF2 and complementary data sets provide new generation libraries shared by these systems.

Innovation studies conducted at CEA concerning future reactors represent a major motivation for further development of the SAPHYR system, for instance for evaluation of a boron-free concept and dedicated control methods, multirecycling of MOX cores, and waste transmutation in PWR.

EPICURE PROGRAMME

The EPICURE programme, conducted in collaboration with EDF and Framatome, was set up in the EOLE and MINERVE reactors at Cadarache, for the purpose of creating a precise experimental data base concerning plutonium recycling in PWR type reactors. This programme was designed to achieve maximum representativity of current and future industrial situations, in order to identify all sources of uncertainty regarding neutronic parameters linked to the safety of reactors of this type (hot spot factor, void effects, etc. The majority of these parameters were thus measured with a very good degree of accuracy, and the resultant experimental data base is making a substantial contribution to qualification of the codes integrated in the SAPHYR system.

5. TYPICAL RESULTS AND IMPROVEMENTS

5.1. Apollo2 code

APOLLO2 is a modular code, in which each module corresponds to a given function:

- access to multi-group nuclear constants,
- geometry and media generation,
- self shielding modelling of the resonances,
- solution of Boltzman's integral equation using collision-probability and S_n integral-differential methods,
- equivalence procedures between different computation methods, for homogenization of the various components of the computation mesh elements.

5.1.1. Nuclear data

APOLLO2 has access to nuclear data libraries from the European JEF2 data bank. The CEA 93 library

exists in 99 and 172 energy group form, and the flexibility of APOLLO2 makes it possible to use different meshes, either with a smaller number of groups, created by the user with a code compression function, or with a high number of groups. Libraries with up to 10.000 groups have been created for dedicated analytical tasks. At this level of energy discretization, the restrictions imposed by the majority of self-shielding models are eliminated, making it possible to conduct "numerical experiments" comparable with those using Monte Carlo methods.

This flexibility in terms of both space and energy, can be used to advantage with the code serving as a reference tool, thus validating the models and computation schemes adopted for industrial studies, as resulting from a compromise between cost, the desired degree of precision, and the area of validity.

The excellent performance of these models was thus demonstrated on the occasion of an international comparison, based on simple configurations restricted to one fuel rod and its associated water, and computed with nuclear constants obtained from the European JEF2 data bank. Differences between the multiplication factor for the APOLLO2 and Monte Carlo MCNP codes for instance are very small. These good results can be attributed to the self-shielding modelling, substantially enhanced by comparison with that for the previous generation, as a result of systematic and detailed analysis of the physical phenomena involved.

The other qualification segment is based on interpretation of critical experiments in a wide range of moderating ratios and constituent materials, and processing of analytical data for fuels irradiated in a PWR. The APOLLO2 code and its associated library give a mean sub-criticality of about 100 pcm for uranium and plutonium thermal reactors, and a super-criticality of about 300 pcm in fast spectrum fuel lattices. The temperature coefficient of the moderator is quantified correctly, and the mean deviation is less than 0.6 pcm/°C, indicating substantial progress with respect to the results obtained with APOLLO1.

5.1.2. Plutonium production balance

Plutonium production in a PWR, using industrial options, is quantified with an uncertainty factor of 1% at current reject irradiation rates. However, greater discrepancies are still observed in the isotopic composition of the plutonium, requiring intensified analysis.

Nevertheless, the improvement in quantification of the plutonium balance is substantial, by comparison with APOLLO1.

Moreover, the accuracy will be improved by future modification in Jef. The redidual discrepancies will be further reduced by methods based on sensitivity studies applied to depletion.

Computation/measurement discrepancy (%) for plutonium production in the Gravelines power station

Burn-up (GWD/t)	35	51
Total plutonium	0.05	0.9
^{239}Pu	2	4.1
^{240}Pu	- 2.8	- 1.8
^{241}Pu	- 1.7	0.3
^{242}Pu	- 3.1	- 9.5

5.1.3. Computation of resonance self-shielding

Modelling of resonance self-shielding with APOLLO2 has achieved substantial progress. Qualification of these models cannot be obtained under experimental conditions. Utilization of reference codes such as the Monte Carlo TRIPOLI code or APOLLO2 itself, with very fine energy meshes, contributes to qualification of self-shielding computation, by performing "numerical experiments" (with a given set of data). It is a first step towards the introduction of assembly-wide and even core-wide Monte Carlo computation by combining probabilistic and deterministic methods.

At the present time, the qualification is excellent for the main heavy isotopes taken individually. Reaction rate in the fuel, as also spatial distribution, are extremely satisfactory, and the centre periphery ratio for this distribution is estimated at better than 2% by comparison with reference calculations.

With fast spectrum configurations, it is necessary to improve the processing of self-shielding by applying sub-group methods, involving the use of

probability tables. This technique has been integrated in APOLLO2.

Satisfactory quantification of plutonium distribution provides data for explaining, on the basis of thermo-mechanical computation, the behaviour of the PWR fuel rod at very high burn up when subjected to a power excursion, for instance in the CABRI rod ejection type experiment (Rim effect).

5.1.4. Collision probability and S_n models

Collision probability fuel assembly computation is generally satisfactory. Reactivity and reaction rates are quantified correctly for a PWR fuel assembly, with or without burnable poison.

Comparison of APOLLO2 S_n methods and the collision probability method confirms that results tend towards the same values when numerical discretization is refined.

Furthermore, S_n methods offer the possibility of correct processing of diffusion anisotropy, for P1 approximation and beyond.

By comparison with the S_n module finite difference method, Sn nodal methods are considerably more efficient from the numerical convergence point of view, and in particular, nodal methods with linear flux representations in the mesh element (CL and LL methods) appear to be particularly suitable for computation of fuel assemblies. Sn nodal precision is better than Sn finite difference computation, as demonstrated by analysis of data from the EPICURE experiments run in the EOLE reactor.

5.1.5. Computation of power distribution and capture rate

Interpretation of EPICURE programme experiment result data demonstrates the capacity of APOLLO2 to handle varied and complex configurations with a good degree of precision.

Poison rod clusters in borated Pyrex, silver-indium-cadmium (AIC) control rod clusters, zoned MOX assemblies, and drained channel configurations are computed with satisfactory precision. All these interpretations demonstrate the good quality of the selected models: collision probability, S_n methods based on the diamond scheme, or CC and LL nodal methods, oriented collision probabilities, and TIBERE model dedicated to streaming determination.

The following table summarises the computed/measured value discrepancies obtained for power distribution after analysis of a number of EPICURE configurations. These are mean, quadratic and maximum discrepancies computed on a centred lattice containing 17 x 17 UO_2 rods, with a cluster of 24 Pyrex rods, or a grey cluster of 12 steel rods and 12 AIC rods. The experiment results simulate a drain-out in a zone limited to 7 x 7 rods, obtained from computation with APOLLO2. TIBERE model for streaming is also included in this table.

Computation/measured value discrepancies for power distribution in the 17 x 17 cluster assembly for a drained 7 x 7 rod zone in the UO_2 core of EPICURE (%)

Configur-ation	Mean discrepancy	Quadratic	Max.
Assembly with no cluster	- 0.4	0.7	- 2.1
Pyrex cluster	- 0.5	1.2	- 2.3
Grey cluster	- 0.3	1.6	- 2.3
Void (7 x 7 alu block)	- 1.3	1.2	- 2.4

5.2. CRONOS2 code

5.2.1. General

The CRONOS code provides all computational resources required for LWR type reactors, HTR, FBR, experimental reactors, dedicated reactors (space, etc.). CRONOS is used for design studies, in-core fuel management studies, on-line monitoring and reactivity accident studies. The equation-solving rapidity of this code opens up possibilities for its utilization as a core model for training simulators. The CRONOS2 code can be used for basic and transient mode operation studies, and handles slow and fast fuel evolution kinetic

problems, using an iterative process for coupling neutronics, FLICA4 core thermohydraulics and FLICA S primary coolant system configurations. All this is possible without restriction on the number of energy groups or spatial meshes.

The power of the numerical models makes it possible to undertake detailed 3D computation at individual fuel rod level, or computation where element size corresponds to fuel assembly section, using the same CRONOS2 code.

The performance of the CRONOS2 numerical methods compares very favourably with that of similar software products. The gain achieved with the MINOS method, in terms of computation time, represents a factor of 10 by comparison with codes based on the state of the art.

CRONOS2 solves diffusion and transport equations for a cylindrical, 1D, 2D or 3D Cartesian, or 2D or 3D hexagonal geometry.

Coupled with the FLICA4 module for two-phase core thermohydraulics, and the FLICA/S module for computation of the primary coolant system, CRONOS2 constitutes a powerful tool for studying complex situations, such as a steam line break or ejection of a control rod cluster.

5.2.2. Solution methods

The CRONOS2 code initially used the finite element primal method, ensuring the continuity of neutron flux at the mesh element boundaries. Subsequently, finite difference methods were introduced, together with particularly efficient coarse mesh rebalancing acceleration techniques.

5.2.3. MINOS method for diffusion problems

Work has also been done on nodal solution methods. Existing models at international level are based on approximation of transverse neutron leakage, for which analytical representation cannot be easily transposed from a Cartesian to a hexagonal geometry. This led to utilization of a dual finite element method. This method has been extended to integrate discontinuity coefficients between elements, and thus handle the problem of homogenizing the various components. The particular choice of a polynomial base, on which the neutron flux and current are broken down, provides very simple matrices with regular structures. The structure of the matrices allow iteration by alternate direction. This method is fully vectorizable, and can be easily converted to parallel form.

This nodal-dual method has been extended to handle kinetic computation tasks.

Comparison of primal and nodal methods on a class 900 PWR xy parabolic, z linear (time in seconds)

	PRIMAL	NODAL	RATIO
RS6000/370	86.9	14.0	6.2
CRAY/C90	25.7	0.7	36.0
xy cubic, z linear (time in seconds)			
	PRIMAL	**NODAL**	**RATIO**
RS6000/370	392	39.0	10.0
CRAY C90	76.0	1.90	39.0

5.2.4. Transport computation

The method used, based on the even flux equation, is an extension of the primal form finite element method. Flux representation is consequently continuous. The degree of the base polynomials can vary up to the fourth order. Angular discretization is based on a discrete ordinate method (S_n), with no restriction on the order of angular representation. The variational system corresponds to a set of N diffusion type systems, coupled uniquely by the impact term.

Incorporated in the CRONOS2 code, the method is operational for PWR computation (integration of thermohydraulic feedback, fuel evolution, adjoint and source computation, etc.). Other methods of the nodal type are in course of development. These include a compound odd flux method, and an

angular Pn method, based on extension of the MINOS solver to provide an accelerator function.

5.2.5. Optimum control method for control rod clusters

For core design studies, control rod cluster control is complicated by the choice of cluster groups to be made, as also determination of cluster movements in accordance with safety criteria. To overcome these constraints, a simulated annealing method has been first developed in collaboration with FRAMATOME, and subsequently the TOPAZE method, used to determine the position of the clusters in order to minimize the power level generated by the hottest fuel rod. TOPAZE is a precise solution method, based on the utilization of influence factors quantified by CRONOS, and determines the optimum offset between the various control rod banks.

6. TEN-YEAR PROSPECTS FOR SOFTWARE DEVELOPMENT

An analysis of development prospects was undertaken in 1991, related to the integration of models and operators contained in SAPHYR (advanced reactor physics software system) and PROMETHEE (dedicated radiation transport, shielding protection and criticality safety software system). This analysis points the way forward in more general terms.

The conclusion reached was that reconfiguration of models and transport equation solver algorithms will be required in the future:

- broadly on the basis of existing operators, (deterministic and probabilistic), with an increased emphasis on Monte Carlo methods;
- on the basis of shared software components and future market standards.

Integration of the transport models available in SAPHYR-PROMETHEE will provide a modelling base, supplied with data essentially by JEF, and completed by adaptation of data and models when required by emerging needs.

As a result of modularity and an "object-operator" methodology, this "model-base" can be used to write down qualified computation schemes, designed for reactor core, protection system, criticality, safety (residual power), fuel cycle and waste computation.

With the sharing of modelling operators in an integrated, modular system, this work will obliterate the traditional divisions:

- between core computation and cell or lattice computation,
- and between the areas of application for the probabilistic and deterministic methods which will be used for the same computation tasks.

This will encourage coupling with other disciplines, via mechanics (CASTEM, PLEXUS) and system thermal-hydraulics (CATHARE), for the study of certain types of criticality accident.

These prospects are integrated in the current thinking at CEA/Directorate for Nuclear Reactors (DRN). In the neutronics field, these prospects point ahead to the SUN operation combining in an overall software architecture the components available in the field of Reactor Physics.